DETERMINATION OF EFFECTIVE ELASTIC COEFFICIENTS USING THE STANDARD MECHANICS APPROACH: APPLICATION TO TRABECULAR BONE TISSUE

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Abstract. The human bone tissue is a natural composite material with a complex microstructure optimized for withstanding functional loads. It is extremely difficult to analyze the mechanical response of the trabecular bone considering each structural entity due to its high degree of heterogeneity. The typical way to overcome this difficulty is to find an equivalent material model that characterizes the average material mechanical behavior in the macroscopic scale. It is presented in this paper a method to compute the macroscopic effective stiffness matrix of the trabecular bone via the so-called standard mechanics approach. To this end, the finite element (FE) method is used to conduct a stress analysis a representative volume element (RVE) of the trabecular microstructure. The FE results are processed in order to compute the local structure tensor $M$, which relates the local tissue strain tensor to the average strain tensor. Finally, the $M$ tensor is used to compute the elastic coefficients for the equivalent continuum material in the macroscopic level. The method is used to obtain the equivalent elastic coefficients for idealized trabecular geometries in 2D. The effect of the RVE size is analyzed and discussed.

Keywords: Bone tissue, effective elasticity tensor, finite element analysis

1. INTRODUCTION

The bone tissue microstructure is optimized for withstanding functional loads. Besides, its reduced weight allows the body to move efficiently with a minimum metabolic cost (Rincón et al., 2004; Keaveny et al., 2002).

The bone tissue possesses hierarchical and heterogeneous structure (Keaveny et al., 2002). This hierarchical structure is usually classified into four levels (Rho et al., 1998): the macrostructural level in which it is possible to distinguish trabecular and cortical bone; the microstructural level in which it is possible to distinguish the Harvesian systems and osteons; the sub-microstructural or nanostructural level where rheological phenomena in the lamellae and collagen fibers take place; and the sub-nanostructural level in which it is possible to distinguish the elemental constituents and the molecular structure.

The mechanical properties of the trabecular bone in combination with its architecture are responsible of the bone resistance and stiffness (Van Rietbergen et al., 1995). Stress and strain fields at the microstructural levels are biologically important, since among other variables, they govern the bone remodeling processes (Cowin, 2007; Currey, 2002). Thus, the understanding of the remodeling mechanisms requires of the knowledge of the stress and strain fields at the microstructural level.

The use of biodegradable scaffolds (or artificial extra-cellular matrices) plays an important role in tissue engineering. One of the crucial requirements for the production of tissue scaffolds are the mechanical properties (Hollister, 2005). Tissue scaffolds must be stiff enough to avoid collapse under loading and compliant enough not to damage surrounding tissue after implantation. In fact, the mechanical properties of a tissue scaffold must match those of the tissue at the site of implantation (Bawolin et al., 2007). Besides in orthopedic treatments the stiffness of a scaffold must reduce in time as the bone recovers its load bearing capacity. Thus, it is important to know the mechanical properties of both, the scaffolds and the trabecular bone, during the remodeling process.

The trabecular tissue can be considered as a linear elastic isotropic material. However, due to its spatial architecture the trabecular bone behaves anisotropically. The behavior of a general elastic material is characterized by the elasticity tensor $E$ in the Hooke law, which is defined in terms of 21 independent elastic constants. The number of independent elastic constants diminishes with the material symmetry. Thus for example, the elastic behavior of orthotropic materials (three planes of symmetry) is defined in terms of 9 independent constants while isotropic materials (infinite planes of symmetry) need of 2 constants only. For materials that exhibit pure orthotropic or higher symmetries Cowin and Mehrabadi (1989) developed a method to determine the principal orthotropic axes from the 21 coefficients of $E$. Although this method allows diminishing the uncertainties associated with the measure of the material texture (or fabric) the actual limitation for its practical application is the current lack of experimental procedures for the determination of the 21 elastic coefficients. In every case the accuracy of the material characterization depends on the quality of the experimental tests and the hypothesis assumed for the material symmetry.

Numerical modeling has emerged as a powerful tool for the mechanical characterization of microstructures. Computational modeling, typically the Finite Element (FE) method, provides the means to assess the effects of the architecture and spatial material distribution of a microstructure on the overall material behavior in the macro scale (say for example, the determination of the elastic constants for the $E$ tensor). However, it is impossible in practice to...
characterize a material by taking into account every microstructural feature. The large mismatch between the micro and macro scale needs of extremely large computer models which can not be solved using the currently available computer facilities (Zohdi and Wriggers, 2005). An alternative procedure for the solution of such a problem is to use representative volume elements (RVE) of the microstructures for the computation of homogenous equivalent material properties in the macroscale. This procedure is usually referred as “homogenization”.

It is presented in this work a method to compute the macroscopic stiffness matrix of trabecular tissue or scaffold via the so-called standard mechanics approach. To this end the FEM is used to conduct stress analysis on RVEs of idealized trabecular geometries in two dimensions. The effect of the RVE size on the value of the computed elastic constants is discussed.

2. METHODS

2.1. The RVE analysis

The analysis is decoupled into two levels which are referred as local and global. The material microstructure is modeled using a RVE at the local level, $i$, while the resulting homogeneous properties are given in the global level, $i-1$. Following Hollister and Kikuchi (1994) the strains computed in the local level, $\varepsilon_i$, can be related to the strains in the global level, $\varepsilon_{i-1}$, using

$$
\varepsilon_i = M_i \cdot \varepsilon_{i-1},
$$

where the subindex $i$ indicates the structural level and $M_i$ is the so-called local structural tensor or strain localization tensor for the $i$-th level. The dimensions of $M$ are $(6 \times 6)$ and $(3 \times 3)$ for three and two dimensional problems respectively. The local structural tensor allows computing the elasticity tensor in the global level, $E_{i-1}$, as follows

$$
E_{i-1} = \frac{1}{V_{rve}} \int_{V_{rve}} E_i M_i dV_{rve},
$$

where $E_i$ is the elasticity tensor at the local level and $V_{rve}$ is the volume of the RVE.

2.2. The standard mechanics approach

The accuracy of the above described procedure depends on the boundary conditions selected for the RVE. In practice, the applied boundary conditions cannot represent all the possible in-situ boundary conditions to which the RVE is subjected within the macroscopic material. The standard mechanics approach uses either constant traction (Reuss) or constant displacement (Voigt) boundary conditions for the RVE. Hill (1952) demonstrated that Voigt boundary conditions result in the upper bound for the elastic constants, while Reuss boundary conditions provide the lower bound.

Not only the boundary conditions but the size of the RVE can affect the homogenization results. The hypothesis of the continuum mechanics holds when the RVE size can be assimilated to a material point when compared to the dimensions of the $i-1$ level. There are two definitions for the RVE (Kouznetsova, 2002): as a statistical representative sample of the microstructure and as the smallest material volume that reproduces the macroscopic material behavior.

Both the above definitions for the RVE present drawbacks. Regarding the first one, it is worth noting that a statistical representative sample of the microstructure, i.e. to include virtually a sampling of all possible microstructural configurations that occur in the material. Clearly, in the case of a non-uniform microstructure such a definition leads to a considerably large RVE, making the numerical modeling of the RVE computationally expensive or even impracticable. The problem with the second definition is that the RVE size could depend on the material behavior and the problem boundary conditions.

A commonly accepted approach to set the size of the RVE in effective property calculations is the Hill’s condition (see Zohdi and Wriggers, 2005; Kouznetsova, 2002). Hill’s condition states that $\langle \sigma \rangle \cdot \langle \varepsilon \rangle = \langle \sigma \cdot \varepsilon \rangle$, where the McCauley brackets stand for the average of the quantity within the RVE. For any perfectly bonded micro heterogeneous body in absence of volume forces two loading states satisfy Hill’s conditions: uniform displacements and uniform tractions boundary conditions.
2.3. Homogenization using the standard mechanics approach

The homogenization procedure by means of the standard mechanics approach uses uniform displacements or uniform tractions boundary conditions for the RVE. Depending on the selected approach the average stress tensor $\langle \sigma \rangle$ or average strain tensor $\langle \varepsilon \rangle$ are calculated using (Hollister and Kikuchi, 1994):

$$\langle \varepsilon \rangle = \frac{1}{V_{rve}} \int \varepsilon dV_{rve} \quad \text{or} \quad \langle \sigma \rangle = \frac{1}{V_{rve}} \int \sigma dV_{rve}, \quad (3)$$

where the stress or strain fields within the RVE can be computed by means of FEA or any other suitable numerical method.

Using the results from Eq. (3), the average or effective stiffness tensor in the global level, $E_{i-1}$, is computed using Eq. (2), and the structural tensor $M_i$ is calculated using the relationship given in Eq. (1). It is worth noting that the computation of $M_i$ requires setting up a system of equations using Eq. (1). To this end, the components of the local strain tensor, $\varepsilon_i$, are obtained by solving a number of linear independent load cases on the RVE (three for the two-dimensional case and six for the three-dimensional case).

3. IMPLEMENTATION

Numerical analyses in this work were performed using the FEA software ABAQUS 6.7 (Simulia, 2007). All the analyses reported are two-dimensional. Among the two sets of boundary conditions for the RVE analysis (see Section 2), uniform displacement one was selected for this work.

Tensor $M_i$ was computed using a subroutine implemented in Matlab (MathWorks, 2004) which solves the system of equations built using Eq. (1). The system of equations was set up using the results of three FE analyses on the RVE: the uniaxial stretching in the horizontal and vertical directions and the in-plane distortion. A second Matlab subroutine was developed to compute $E_{i-1}$ from $M_i$ using Eq. 2.

The models were constructed using a basic repeating unit (or cell) composed by trabecular tissue and voids. In order to verify the Hill condition the RVE must be perfectly bonded, so that, not only the trabecular tissue but also the void portion of the domain was discretized. In this way the RVE can be solved using a standard FEM code. The void portion of the domain was assigned the properties of a homogeneous compressible linear elastic material with a negligible Young modulus when compared to that of the trabecular tissue, see Tab. 1. Models were discretized using second-order triangular elements (Abaqus element code CPS6M). Deformation results were reported at the element centroids. The FE meshes were refined adaptively using the mesh optimization facility in ABAQUS. Meshes were optimized using the energy density criterion with a maximum allowable error of 5%. In addition the Hill’s condition was also check. The error for the Hill’s condition was found always below 5%.

<table>
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<tr>
<th>Property</th>
<th>Tissue</th>
<th>Void</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young Modulus</td>
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<td>$10^7$ Mpa</td>
</tr>
<tr>
<td>Poisson Ratio</td>
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<td>0</td>
</tr>
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4. STUDY CASES

The above introduced methodology was applied to homogenize the elastic properties of two idealized trabecular geometries in two dimensions. In order to assess the effect of the RVE size on the computed results, a number of RVE of square shape with 1, 2, 3, 4 and 5 cells per side were solved.

4.1. Square cell with a circular void

The first example consists in a square cell with a circular void. The solid volume fraction is 30%. The discretization of the repeating unit was built using 12300 elements, see Fig. 1.a. The smallest and the biggest RVEs were also analyzed by a direct method in order to obtain an estimate of the overall shear modulus $G$. To this end, displacements in one side were constrained and a known tangential displacement was applied to the opposite side.
4.2. Diamond-shape trabeculae

The second example consists of a diamond-shape trabeculae with solid volume fraction of 31.67%. A finite element mesh consisting of 1472 elements was employed to build the five RVEs, see Fig. 1.b.

![Figure 1. Twenty five-cell RVE and detail of the repeating unit for: (a) the square cell with a circular void, (b) the diamond-shape trabeculae.](image)

Table 2. Results for the square cell with a circular void

<table>
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<th>Component</th>
<th>Cells per side</th>
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<tbody>
<tr>
<td></td>
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</tr>
<tr>
<td>$C_{11}$</td>
<td>0.164</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>0.113</td>
</tr>
<tr>
<td>$C_{21}$</td>
<td>0.112</td>
</tr>
<tr>
<td>$C_{22}$</td>
<td>0.164</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td>$8.114 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 3. Results for the two dimensional diamond-shape trabeculae

<table>
<thead>
<tr>
<th>Component</th>
<th>Cells per side</th>
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<tbody>
<tr>
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<td>$C_{22}$</td>
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</tr>
<tr>
<td>$C_{33}$</td>
<td>0.167</td>
</tr>
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</table>

5. RESULTS

Tables 2 and 3 show the normalized results for the components of the tensor $E$, $C_{ij} = E_{ij}/Y$ (where $Y$ is the tissue Young modulus) computed using the homogenization method. These results are plotted in Fig. 2 as a function of the RVE size expressed in terms of the number of cells per side. Due to the restrictions in space those components equal to zero or smaller than $10^{-8}$ are not reported. The normalized overall shear modulus computed for the square cell with a circular void using the direct method are $G/Y= 2.3 \times 10^{-3}$ and $3.9 \times 10^{-3}$ for the smallest and the biggest RVE sizes respectively.
Figure 2. Evolution of the normalized stiffness tensor coefficients, \( C_{ij}/Y \), as a function of the RVE size expressed in terms of the number of cells per side. Square cell with a circular void (left) and diamond-shape trabeculae (right).

6. DISCUSSION

The existence of symmetries planes can be inferred from direct inspection of the values reported in Tab. 2 and Tab. 3. Symmetry planes are found to be coincident with the adopted loading directions. The values of the pairs of components \( C_{11} - C_{22} \) and \( C_{12} - C_{21} \) behave the same and they both exhibit a convergent behavior with the increment of the RVE size (see Fig. 2). The square cell with the circular void converges to a lower limit, while the diamond-shape trabeculae seems to converge to an upper limit. On the other hand, the components \( C_{33} \) remain constant and independent of the RVE size. Similar results were reported by Hollister and Kikuchi (1992) for the geometry of the square cell with a circular void.

Shear modulus determined by a direct method for the square cell with a circular void are 0.57 and 0.96 times the value estimated by the homogenization procedure for the smallest and the biggest RVEs respectively. The \( G \) modulus seems to converge to the homogenization value as the RVE size increases, see Fig. 3.

Figure 3. Comparison of shear modulus \( G \) determined by two methods.

Results in Figs. 2 and 3 show the strong influence of the RVE size on the values of the elasticity tensor coefficients. The increment of the RVE size for the square cell with a void model (beyond five cells per side) does not produce an abrupt change of \( C_{11} \) and \( C_{22} \) as it does it for the smaller RVEs. In contrast, the upper limit is not evident even for the biggest RVE for the diamond-shape trabeculae model. This behavior can be explained by the fact that the fluctuations in the boundary field relative to the size of a RVE are smaller as the size of the model increases. A RVE size with four cells per side make the boundary fluctuations small enough for the square cell with a void, but for the diamond-shape trabeculae it is necessary to further increase the RVE size.
7. CONCLUSIONS

A homogenization method to calculate the coefficients of the elasticity tensor $E$ in a heterogeneous material using the standard mechanics approach was applied to idealized models of trabecular bone.

Using this method the components of the elasticity tensor for trabecular bone material can be estimated without the need for experimental (physical) tests, and without any assumption about the elastic symmetries of the material at the macroscopic level.

Two examples were analyzed: the square cell with a circular void and the diamond-shape trabeculae. The coefficients of the elasticity tensor $E$ converge asymptotically to limiting values as the size of the RVE increases. The size of the RVE diminishes the influence of the boundary field fluctuations. While a RVE size with four cells per side was found enough to minimize the influence of the deformation fluctuations in the square cell with a circular void model, a bigger RVE is necessary for the diamond-shape trabeculae model.

The homogenization method does not allow for an a priori estimate of the RVE size even when dealing with a microstructure consisting of a repeating unit or cell. However, this is not a drawback when dealing with real trabecular bone which exhibits a non-periodic microstructure.

In future works the method will be used to find the size of the RVE in specific regions of a bone by using images of real trabeculii obtained via microcomputed tomography scans.

8. ACKNOWLEDGEMENTS

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9. REFERENCES


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